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A SUBROUTINE FOR THE EQUATION OF STATE OF AIR

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by

L. R. Doan
1/Lt USAF

G. H. Nickel
1/Lt USAF

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ABSTRACT

A "semi-physical fit" to the equation of state of air is generated from tabulated values. The form is


$$P = (\gamma - 1) \rho \epsilon$$

$$\gamma = \gamma(p, \epsilon)$$

$$\rho = \text{mass/volume}$$

$$\epsilon = \text{energy/mass}$$

A listing of the FORTRAN subroutine AIR is given, as well as a graph of tabulated and subroutine-computed values of $(\gamma - 1)$.


DAVID R. JONES
Colonel USAF
Chief, Physics Branch

1. A SUBROUTINE FOR THE EQUATION OF STATE OF AIR.

Computer calculations of expanding fireballs in the atmosphere require some form of equation of state for air which is valid over many orders of magnitude variation in density and energy. Many SHELL calculations have been made using an equation of state which appears much too simple. However, these calculations have given results for fireball growth and rise which agree amazingly well with experiments. Unfortunately, these results cannot be expected to give reliable pictures of temperature within the fireball simply because of the inadequacies in the equation of state. The distribution of temperatures within the fireball is extremely important in fireball calculations since it determines electron density. This note describes an interim effort to provide a good equation of state for computer codes.

Previous SHELL calculations have used γ_1 if $\epsilon < \epsilon_{ion}$, or γ_2 if $\epsilon > \epsilon_{ion}$, where ϵ_{ion} is an input value. The two values of γ were chosen before each problem by referring to the real equations of state. We decided to try a simple fit to $(\gamma-1)$ for an ideal gas equation of state, as computed by NBS.¹ The variables which define this equation of state are chosen as material density and energy density (per mass) rather than density and temperature. Hydrodynamics calculations always involve material and energy densities, and temperature is not used as an independent variable.*

The first look at possible forms for this fit was directed to the density dependence. Crossplots of $(\gamma-1)$ versus density for different energies revealed an approximate behavior of the form

*This fact rules out the use of analytic fits to the equation of state of air using temperature as an independent variable as in RAND RM-2249 by Harold Brode.

$$(\gamma-1) = \left[\gamma(\rho_0, \epsilon) - 1 \right] \left(\frac{\rho}{\rho_0} \right)^{\alpha(\epsilon)}$$

ρ_0 = sea level density

$$= 1.293 \times 10^{-3} \text{ gm/cm}^3$$

The exponent α determines density spreading, and is zero below $\epsilon = 1$ jerk per megagram or 10^{10} ergs per gram. Above $\epsilon = 1$, $\alpha(\epsilon)$ is roughly linear in $\log(\epsilon)$ (see figure 1). Assuming the density dependence discovered, the problem reduces to finding a fit for $\gamma(\rho_0, \epsilon)$. The energy dependence of $(\gamma-1)$ is influenced by the dissociation of the major constituent molecules (only oxygen and nitrogen contribute much to the thermodynamic properties). There are four different "regimes" which are defined below:

- I. Nothing dissociated $0 < \epsilon < \sim 5$
- II. Only oxygen dissociated $\sim 9 < \epsilon < \sim 30$
- III. Everything dissociated $\sim 50 < \epsilon < \sim 150$
- IV. Electrons contributing $\sim 150 < \epsilon < \infty$

Each "regime" has its own energy dependence, and the thermodynamic properties of air are those of whichever "regime" represents the composition of the air. Transitions in properties are made as the composition changes.

Regimes I and II are affected primarily by the increasing occupation of vibrational and electronic levels of undissociated molecules. The energy dependence of regime III is due to increasing occupation of electronic energy levels, and regime IV is the threshold of the Fermi-Thomas description.*

Thermodynamically, $(\gamma-1)$ is the same as $2/n$, where n is the number of degrees of freedom. In a gas whose molecules or atoms have internal

* See, for instance, "LA-2124" on TFD theory.

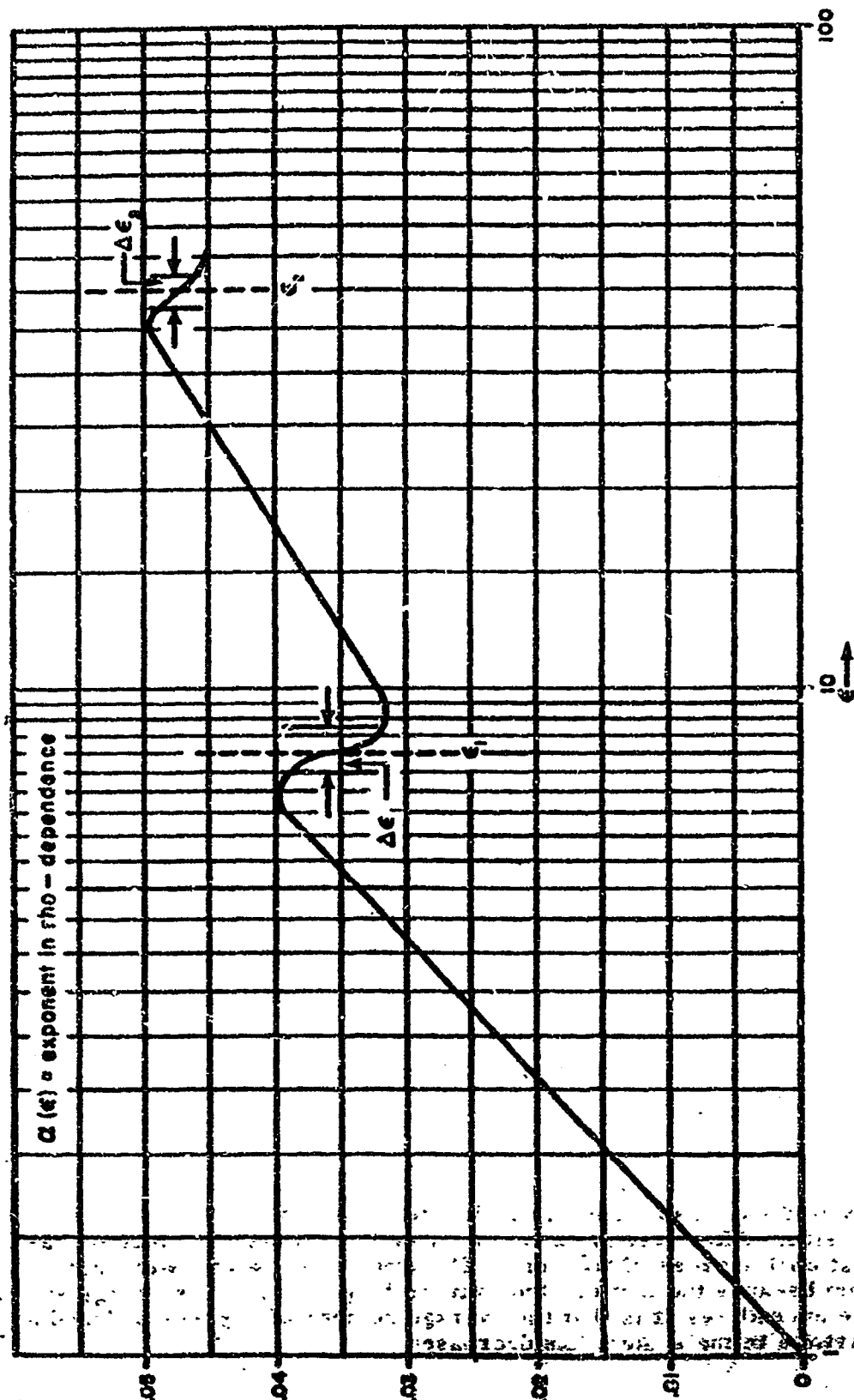


Figure 1. Sketch of $\alpha(\epsilon)$ vs. ϵ

structure, n need not be an integer. For example, an oxygen or nitrogen molecule is rotating but not vibrating at room temperature, and has an n of $3 + 2 = 5$. An energy increase will make n change from 5 to 7 (although the molecule may dissociate before n reaches 7). Regimes I and II represent this change, plus electronic excitation, for O_2 and N_2 .

The hump of increasing γ at $\epsilon = 8$ is due to the decrease in n for oxygen from 7 to 3 as the molecules dissociate and can no longer rotate or vibrate. A similar increase in γ occurs as the nitrogen dissociates, and again as the electrons* (with no internal energy levels) become numerous.

A fit to $\gamma(\rho_0, \epsilon)$ for the entire interval could be generated by a large polynomial, but there is more physical significance in a series of experimental fits for each regime which are "turned on and off" as the composition changes.

In practice, "on and off switches" of the form

$$f_i = \frac{1}{1 + \exp\left(\frac{\epsilon - \epsilon_0}{\Delta\epsilon}\right)}$$

have been found to cause suitable transitions at the "humps" between functions which have been chosen to fit the data closely between "humps." These switches have values from 0 to 1 with a certain width ($\sim 6\Delta\epsilon$) centered about the energy ϵ_0 and have no particular physical significance in this work. It seems reasonable to suppose, however, that ϵ_0 is related in some way to the dissociation energy and $\Delta\epsilon$ to the dissociation equilibrium constant.

*An excited atom has many available energy states in which its electrons may reside. After leaving the atom, upon ionization, the electron has 3 translational degrees of freedom. The atom is left with fewer degrees of freedom because the lost electron will no longer occupy its energy states and the overall result is that the average number of degrees of freedom per particle in the system has decreased.

If we choose to fit the data with exponentials of the form

$$Ae^{-\epsilon/\epsilon_2}$$

then our method leads us to the following form for the equation of state:

$$P = (\gamma - 1) p \epsilon$$

$$\gamma - 1 = \left\{ a + b e^{-\epsilon/\epsilon_1} f_1 + c e^{-\epsilon/\epsilon_2} (1 - f_1) + d e^{-\epsilon/\epsilon_3} f_2 + g f_3 \right\} \frac{p}{p_0} a(\epsilon)$$

$$a(\epsilon) = a_1 f_1 + a_2 (1 - f_1) (1 - f_2) + a_3 f_2$$

(We might expect the density spread to be different for each regime.)

$$a_1 = \beta_1 \log \epsilon; a_2 = \beta_2 \log \epsilon; a_3 = \beta_3$$

The "switches" are given by

$$\text{(Oxygen)} \quad f_1 = \frac{1}{e^{\left(\frac{\epsilon - \epsilon_{0 \rightarrow 20}}{\Delta \epsilon_{0 \rightarrow 20}} \right)} + 1}$$

$$\text{(Nitrogen)} \quad f_2 = \frac{1}{e^{\left(\frac{N_2 - 2N}{\Delta N_{2 \rightarrow 2N}} \right)} + 1}$$

$$\text{(Electrons)} \quad \ell_3 = \frac{1}{\epsilon \left(\frac{z_e - \epsilon}{\Delta \epsilon_e} \right) + 1}$$

This is still not complicated enough to give a close description, since each transition energy and width decreases with decreasing density. This density dependence was represented by

$$\epsilon_{0 \rightarrow 20} = \epsilon_0 \left(\frac{\rho}{\rho_0} \right)^{\delta} \quad \text{etc. and}$$

$$\Delta \epsilon_{0 \rightarrow 20} = \Delta \epsilon_0 \left(\frac{\rho}{\rho_0} \right)^{\eta} \quad \text{etc.}$$

The constants were evaluated by a very straightforward technique: guess values, plot curves, guess new values. Toward the end, the curves were computed by machine, but the same technique was followed. After many tedious attempts, each coming a little closer, it was decided to stop, call this an interim equation of state, and continue with more dignified techniques. The results of the program to date indicate that the approach is worthwhile. Rather than list values for each constant (which will probably change later) we list a subroutine (appendix I) in FORTRAN which will produce $(\gamma-1)$ with an error generally from 0-2 percent with occasional increases to 5 percent. The tabulated and fitted values of $(\gamma-1)$ are given in figure 2. The equations with numbers appear in appendix II. Temperatures above 1.5 ev were not given much consideration, since radiation transport influences things above that temperature, and our planned application is for "simple" hydrodynamics only. It may be possible to continue the description of regime IV to infinite energy by using a TFD equation of state.

Further applications of this fit are numerous. With this equation of state, one can use SHIELD for fireball computations and probably believe the temperatures. The same form may hold for other gases and vapors.

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Lt. J. D. Garcia has suggested that altering the energies of transition may account for nonequilibrium effects in dissociation as the fireball expands rapidly. This seems quite possible, once it can be determined how to compute the new transition energy. Techniques to determine the coefficients from theoretical methods (as opposed to curve-fitting) may uncover new freedom in generating equations of state for other gases.

Finally, the continuation of this work to include equations of state for earth, fire, and water will allow calculations for all possible substances.

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Appendix I

A LISTING OF THE FORTRAN SUBROUTINE AIR

Appendix II

The equation with the present numbers:

$$\gamma - 1 = \left\{ .161 + .255 e^{-\epsilon/4.46} f_1 + .280 e^{-\epsilon/6.63} (1 - f_1) + \right. \\ \left. .137 e^{-\epsilon/25.5} f_2 + .050 f_3 \right\} \left(\frac{p}{p_0} \right)^{\alpha(\epsilon)}$$

$$\alpha(\epsilon) = .048 f_1 \log_{10} \epsilon + .032 (1 - f_1) (1 - f_2) \log_{10} \epsilon + .045 f_2$$

$$f_1 = \frac{1}{e \frac{\epsilon - \epsilon_1}{\Delta \epsilon_1} + 1}$$

$$\epsilon_1 = 8.5 + .357 \log_{10} \left(\frac{p}{p_0} \right)$$

$$\Delta \epsilon_1 = .975 \left(\frac{p}{p_0} \right)^{.05}$$

$$f_2 = \frac{1}{e \frac{\epsilon_2 - \epsilon}{\Delta \epsilon_2} + 1}$$

$$\epsilon_2 = 45. \left(\frac{p}{p_0} \right)^{.0157}$$

$$\Delta \epsilon_2 = 4.0 \left(\frac{p}{p_0} \right)^{.085}$$

$$f_3 = \frac{1}{e \frac{\epsilon_3 - \epsilon}{\Delta \epsilon_3}}$$

$$\epsilon_3 = 160.$$

$$\Delta \epsilon_3 = 6.$$

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1. Hilsenrath, Klein, and Woolley, Tables of Thermodynamic Properties of Air Including Dissociation and Ionization from 1,500°K to 15,000°K, NBS, AEDC TR 59-20, December 1959.
2. Gilmore, F. R., Equilibrium Composition and Thermodynamic Properties of Air to 24,000°K, RAND, RM-1543, 24 August 1955.

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